```
C:\stnweb\Queries\1a.str
chain nodes :
```

```
11 12
ring nodes:
    1 2 3 4 5 6 7 8
ring/chain nodes:
    13
chain bonds:
    1-11 2-13 11-12
ring bonds:
    1-2 1-5 2-3 3-4 4-5 4-6 5-8 6-7 7-8
exact/norm bonds:
    1-2 1-5 1-11 2-3 2-13 3-4 4-5 4-6 5-8 6-7 7-8 11-12
solated ring systems:
    containing 1:
61:C,N
```

latch level :
 1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 11:CLASS 12:CLASS
 13:CLASS

| * * *           | * *  | * *          | * *   | * Welcome to STN International * * * * * * * * *                           |  |  |  |  |  |  |  |  |
|-----------------|------|--------------|-------|--|--|--|--|--|--|--|--|--|
| NEWS            | 1    |              |       | Web Page URLs for STN Seminar Schedule - N. America                        |  |  |  |  |  |  |  |  |
| NEWS            |      |              |       | "Ask CAS" for self-help around the clock                                   |  |  |  |  |  |  |  |  |
| NEWS            |      | SEP          | 09    | CA/CAplus records now contain indexing from 1907 to the                    |  |  |  |  |  |  |  |  |
|                 |      |              |       | present  |  |  |  |  |  |  |  |  |
| NEWS            | 4    | DEC          | 8 0   | INPADOC: Legal Status data reloaded  |  |  |  |  |  |  |  |  |
| NEWS            | 5    | SEP          | 29    | DISSABS now available on STN   |  |  |  |  |  |  |  |  |
| NEWS            | 6    | OCT          | 10    | PCTFULL: Two new display fields added                                      |  |  |  |  |  |  |  |  |
| NEWS            | 7    | OCT          | 21    | BIOSIS file reloaded and enhanced  |  |  |  |  |  |  |  |  |
| NEWS            | 8    | OCT          | 28    | BIOSIS file segment of TOXCENTER reloaded and enhanced                     |  |  |  |  |  |  |  |  |
| NEWS            | 9    | NOA          | 24    | MSDS-CCOHS file reloaded   |  |  |  |  |  |  |  |  |
| NEWS            |      | DEC          | 8 0   | CABA reloaded with left truncation   |  |  |  |  |  |  |  |  |
| NEWS            |      | DEC          | 8 0   | IMS file names changed   |  |  |  |  |  |  |  |  |
| NEWS            | 12   | DEC          | 09    | Experimental property data collected by CAS now available in REGISTRY      |  |  |  |  |  |  |  |  |
| NEWS            | 13   | DEC          | 09    | STN Entry Date available for display in REGISTRY and CA/CAplus             |  |  |  |  |  |  |  |  |
| NEWS            | 14   | DEC          | 17    | DGENE: Two new display fields added  |  |  |  |  |  |  |  |  |
| NEWS            | 15   | DEC          | 18    | BIOTECHNO no longer updated  |  |  |  |  |  |  |  |  |
| NEWS            | 16   | DEC          | 19    | CROPU no longer updated; subscriber discount no longer                     |  |  |  |  |  |  |  |  |
|                 |      |              |       | available  |  |  |  |  |  |  |  |  |
| NEWS            | 17   | DEC          | 22    | Additional INPI reactions and pre-1907 documents added to CAS databases    |  |  |  |  |  |  |  |  |
| NEWS            | 18   | DEC          | 22    | IFIPAT/IFIUDB/IFICDB reloaded with new data and search fields              |  |  |  |  |  |  |  |  |
| NEWS            |      |              | 22    |  |  |  |  |  |  |  |  |  |
| NEWS            | 20   | JAN          | 27    | Source of Registration (SR) information in REGISTRY updated and searchable |  |  |  |  |  |  |  |  |
| NEWS            | 21   | JAN          | 27    | A new search aid, the Company Name Thesaurus, available in CA/CAplus       |  |  |  |  |  |  |  |  |
| NEWS            | 22   | FEB          | 05    | German (DE) application and patent publication number format changes       |  |  |  |  |  |  |  |  |
| NEWS            | EXP  | RESS         |       | CEMBER 28 CURRENT WINDOWS VERSION IS V7.00, CURRENT                        |  |  |  |  |  |  |  |  |
|                 |      |              |       | CINTOSH VERSION IS V6.0b(ENG) AND V6.0Jb(JP),                              |  |  |  |  |  |  |  |  |
| MERIC           |      |              |       | CURRENT DISCOVER FILE IS DATED 23 SEPTEMBER 2003                           |  |  |  |  |  |  |  |  |
| NEWS            |      |              |       | N Operating Hours Plus Help Desk Availability                              |  |  |  |  |  |  |  |  |
| NEWS            |      |              |       | neral Internet Information   |  |  |  |  |  |  |  |  |
| NEWS            |      | _            |       | come Banner and News Items   |  |  |  |  |  |  |  |  |
| NEWS            |      | 1E           |       | sect Dial and Telecommunication Network Access to STN                      |  |  |  |  |  |  |  |  |
| NEWS            | WWW  |              | CAS   | S World Wide Web Site (general information)                                |  |  |  |  |  |  |  |  |
| Enter<br>specif | NEWS | fol<br>copic | llowe | ed by the item number or name to see news on that                          |  |  |  |  |  |  |  |  |

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FILE 'HOME' ENTERED AT 20:57:26 ON 02 MAR 2004

=> file reg

SINCE FILE COST IN U.S. DOLLARS TOTAL ENTRY SESSION FULL ESTIMATED COST 0.21 0.21

FILE 'REGISTRY' ENTERED AT 20:57:31 ON 02 MAR 2004

USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT. PLEASE SEE "HELP USAGETERMS" FOR DETAILS.

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Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 1 MAR 2004 HIGHEST RN 656797-92-1 DICTIONARY FILE UPDATES: 1 MAR 2004 HIGHEST RN 656797-92-1

TSCA INFORMATION NOW CURRENT THROUGH JULY 14, 2003

Please note that search-term pricing does apply when conducting SmartSELECT searches.

Crossover limits have been increased. See <a href="HELP CROSSOVER">HELP CROSSOVER</a> for details.

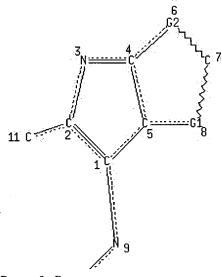
Experimental and calculated property data are now available. For more information enter <u>HELP PROP</u> at an arrow prompt in the file or refer to the file summary sheet on the web at: http://www.cas.org/ONLINE/DBSS/registryss.html

=> L1 STRUCTURE UPLOADED

=> d 11 L1 HAS NO ANSWERS L1 STR

C 14 S 15 N 16

C 12 N 13 Page 1-A

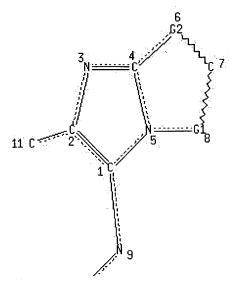


Page 1-B



VAR G1=12/13 VAR G2=14/15/16

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             AT
NSPEC
       IS R
                AT
             AT
AT
NSPEC IS R
NSPEC IS R
NSPEC IS R
               AΤ
NSPEC IS R
                AT
NSPEC IS R
                AT
NSPEC IS R
NSPEC IS C
                 AΤ
NSPEC
       IS C
                 AT
                     10
NSPEC
       IS RC
                 AT 11
DEFAULT MLEVEL IS ATOM
MLEVEL IS CLASS AT
                      9 10 11
DEFAULT ECLEVEL IS LIMITED
GRAPH ATTRIBUTES:
RSPEC I
NUMBER OF NODES IS
STEREO ATTRIBUTES: NONE
=> s 11
SAMPLE SEARCH INITIATED 20:58:01 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 236 TO ITERATE
                    236 ITERATIONS
100.0% PROCESSED
                                                             0 ANSWERS
SEARCH TIME: 00.00.01
FULL FILE PROJECTIONS: ONLINE **COMPLETE**
                       BATCH **COMPLETE**
PROJECTED ITERATIONS:
                             3799 TO 5641
PROJECTED ANSWERS:
                                0 TO
             O SEA SSS SAM L1
L2
=> s 11 full
THE ESTIMATED SEARCH COST FOR FILE 'REGISTRY' IS 155.00 U.S. DOLLARS
DO YOU WANT TO CONTINUE WITH THIS REQUEST? (Y) /N or END:y
FULL SEARCH INITIATED 20:58:04 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 4516 TO ITERATE
100.0% PROCESSED
                   4516 ITERATIONS
                                                             0 ANSWERS
SEARCH TIME: 00.00.01
             0 SEA SSS FUL L1
L3
L4
       STRUCTURE UPLOADED
=> d 14
L4 HAS NO ANSWERS
L4
               STR
C 14 S 15 N 16
C 12 N 13
Page 1-A
```



Page 1-B

10 Page 2-B VAR G1=12/13

VAR G1=12/13 VAR G2=14/15/16

NODE ATTRIBUTES:

NSPEC IS R AT1 IS R ATNSPEC NSPEC IS R ATNSPEC IS R ATNSPEC IS R ATNSPEC IS R ATNSPEC IS R AT NSPEC IS R AT8 NSPEC IS C AT 9 NSPEC IS C AT10 IS RC AT**NSPEC** 11 DEFAULT MLEVEL IS ATOM

MLEVEL IS CLASS AT 9 10 11

DEFAULT ECLEVEL IS LIMITED

**GRAPH ATTRIBUTES:** 

RSPEC I

NUMBER OF NODES IS 16

STEREO ATTRIBUTES: NONE

## => s 14

SAMPLE SEARCH INITIATED 20:58:58 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 219 TO ITERATE

100.0% PROCESSED 219 ITERATIONS

217 11110

6 ANSWERS

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE \*\*COMPLETE\*\*

BATCH \*\*COMPLETE\*\*

PROJECTED ITERATIONS:

3493 TO 5267

PROJECTED ANSWERS:

6 TO 266

6 SEA SSS SAM L4

=> s 14 full

THE ESTIMATED SEARCH COST FOR FILE 'REGISTRY' IS 155.00 U.S. DOLLARS DO YOU WANT TO CONTINUE WITH THIS REQUEST? (Y)/N or END:y FULL SEARCH INITIATED 20:59:02 FILE 'REGISTRY' FULL SCREEN SEARCH COMPLETED -4744 TO ITERATE

100.0% PROCESSED 4744 ITERATIONS 86 ANSWERS

SEARCH TIME: 00.00.01

1.6

86 SEA SSS FUL L4

=> file hcaplus

COST IN U.S. DOLLARS

SINCE FILE TOTAL ENTRY

SESSION

311.26

311.47

FULL ESTIMATED COST

FILE 'HCAPLUS' ENTERED AT 20:59:07 ON 02 MAR 2004 USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT. PLEASE SEE "HELP USAGETERMS" FOR DETAILS. COPYRIGHT (C) 2004 AMERICAN CHEMICAL SOCIETY (ACS)

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FILE COVERS 1907 - 2 Mar 2004 VOL 140 ISS 10 FILE LAST UPDATED: 1 Mar 2004 (20040301/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> s 16

16 L6

=> s 16/thu

16 L6

574682 THU/RL

L8

4 L6/THU

(L6 (L) THU/RL)

=> d 18, ibib abs fhitstr, 1-4

L8 ANSWER 1 OF 4 HCAPLUS COPYRIGHT 2004 ACS on STN

Full Citing References ACCESSION NUMBER:

DOCUMENT NUMBER:

2003:507684 HCAPLUS

139:85530

TITLE:

Preparation of C1 to c4 side-chain modified

INVENTOR (S):

nodulisporic acid analogs as anthelmintic agents Shih, Thomas; Colletti, Steven L.; Fisher, Michael H.;

Meinke, Peter T.; Kuo, Howard C. H.; Chakravarty, Prasun K.; Wyvratt, Matthew J.; Tyagarajan, Sriram;

Berger, Richard

PATENT ASSIGNEE(S):

Merck & Co., Inc., USA

SOURCE:

U.S., 57 pp. CODEN: USXXAM

DOCUMENT TYPE:

Patent

LANGUAGE:

English

FAMILY ACC. NUM. COUNT:

PATENT INFORMATION:

| PATENT | NO. |
|--------|-----|
|        |     |

KIND DATE APPLICATION NO. DATE

US 6586452

20030701 В1

\_\_\_\_\_\_ US 2001-901266

I

Π

20010709 20000714

PRIORITY APPLN. INFO.:

US 2000-218398P P

OTHER SOURCE(S):

MARPAT 139:85530

GΙ

Me Me Me Me Me Me R3 R2 R1 
$$\stackrel{\text{Me}}{\underset{\text{CH}_2}{\text{He}}}$$
  $\stackrel{\text{Me}}{\underset{\text{R5}}{\text{He}}}$   $\stackrel{\text{Me}}{\underset{\text{R5}}{\text{He}}}$   $\stackrel{\text{R6}}{\underset{\text{R5}}{\text{R7}}}$ 

Nodulisporic acid derivs., such as I [R1 = H, alkyl, alkenyl, alkynyl, AΒ cycloalkyl, aryl, heterocyclyl; R2-R4 = (substituted) OH; R1R2 = O; R5 = H, (substituted) OH; R4R5 = O; R6-R8 = H, alkyl, alkenyl, aryl, cycloalkyl, halo, CN acyl, amino, etc.] were prepd. The compds. were acaricidal, antiparasitic, insecticidal and anthelmintic agents. Thus, nodulisporic acid deriv. II was prepd. via a multistep synthetic sequence starting from nodulisporic acid A, N-methylhydroxylamine hydrochloride and N-phenyl-maleimide.

IT 552836-27-8P

RL: AGR (Agricultural use); PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(prepn. of C1 to c4 side-chain modified nodulisporic acid analogs as anthelmintic agents)

552836-27-8 HCAPLUS RN

1H-Benz[6,7]indeno[1,2-b]pyrano[3',4':4,5]cyclopenta[1,2-f]pyrrolo[3,2,1-CN hi]indol-14(15H)-one, 4-[(1E)-2-[5-[(1,1-dimethylethyl)amino]imidazo[1,2b]thiazol-6-yl]ethenyl]-2,3,4,4a,5,6,6a,7,10,12,12a,13,16b,16ctetradecahydro-3,13-dihydroxy-4,10,10,12,12,16b,16c-heptamethyl-15-(1methylethenyl) -, (3S,4S,4aR,6aS,12aR,13S,15S,16bS,16cS) - (9CI) (CA INDEX NAME)

Absolute stereochemistry.

Double bond geometry as shown.

PAGE 1-B

N

REFERENCE COUNT:

6 THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L8 ANSWER 2 OF 4 HCAPLUS COPYRIGHT 2004 ACS on STN

Full Clang Text References

ACCESSION NUMBER:

2001:798222 HCAPLUS

DOCUMENT NUMBER:

135:344484

TITLE:

Preparation of N-acylimidazopyridineamine chlorides

and analogs as  $\mu$ -opiate receptor ligands

INVENTOR(S):

Gerlach, Matthias; Maul, Corinna

PATENT ASSIGNEE(S):

Gruenenthal G.m.b.H., Germany

SOURCE:

PCT Int. Appl., 83 pp.

CODEN: PIXXD2

DOCUMENT TYPE:

Patent German

LANGUAGE:

German

FAMILY ACC. NUM. COUNT:

PATENT INFORMATION:

| PATENT NO.    |             |             |     | KI          | KIND DATE   |     |     |                         | APPLICATION NO. DATE      |     |     |     |     |     |          |     |     |
|---------------|-------------|-------------|-----|-------------|-------------|-----|-----|-------------------------|---------------------------|-----|-----|-----|-----|-----|----------|-----|-----|
|               |             | - <b></b> - |     |             |             |     |     |                         | -                         |     |     |     |     |     | <b>-</b> |     |     |
| WO 2001081344 |             |             | 44  | A1 20011101 |             |     |     | WO 2001-EP3772 20010403 |                           |     |     |     |     |     |          |     |     |
|               | W:          | ΑE,         | AG, | AL,         | AM,         | ΑT, | AU, | ΑZ,                     | BA,                       | BB, | BG, | BR, | BY, | BZ, | CA,      | CH, | CN, |
|               |             | CO,         | CR, | CU,         | CZ,         | DK, | DM, | DZ,                     | EE,                       | ES, | FI, | GB, | GD, | GE, | GH,      | GM, | HR, |
|               |             | ΗU,         | ID, | IL,         | IN,         | IS, | JP, | KE,                     | KG,                       | KΡ, | KR, | ΚZ, | LC, | LK, | LR,      | LS, | LT, |
|               |             | LU,         | LV, | MA,         | MD,         | MG, | MK, | MN,                     | MW,                       | MX, | MZ, | NO, | ΝZ, | PL, | PT,      | RO, | RU, |
|               |             | SD,         | SE, | SG,         | SI,         | SK, | SL, | ТJ,                     | TM,                       | TR, | TT, | TZ, | UA, | UG, | US,      | UZ, | VN, |
|               |             | YU,         | ZA, | ZW,         | AM,         | ΑZ, | BY, | KG,                     | ΚZ,                       | MD, | RU, | TJ, | TM  |     |          |     |     |
|               | RW:         | GH,         | GM, | KE,         | LS,         | MW, | MZ, | SD,                     | SL,                       | SZ, | TZ, | UG, | ZW, | ΑT, | BE,      | CH, | CY, |
|               |             | DE,         | DK, | ES,         | FI,         | FR, | GB, | GR,                     | ΙE,                       | IT, | LU, | MC, | NL, | PT, | SE,      | TR, | BF, |
|               |             | ВJ,         | CF, | CG,         | CI,         | CM, | GΑ, | GN,                     | GW,                       | ML, | MR, | NE, | SN, | TD, | TG       |     |     |
| DE            | DE 10019714 |             |     |             |             |     |     |                         | DE 2000-10019714 20000420 |     |     |     |     |     |          |     |     |
| EP            | EP 1274709  |             |     |             | A1 20030115 |     |     |                         | EP 2001-931560 20010403   |     |     |     |     |     |          |     |     |
|               | R:          | AT,         | BE, | CH,         | DE,         | DK, | ES, | FR,                     | GB,                       | GR, | IT, | LI, | LU, | NL, | SE,      | MC, | PT, |
|               |             | ΙE,         | SI, | LT,         | LV,         | FΙ, | RO, | MK,                     | CY,                       | ΑL, | TR  |     |     |     |          |     |     |

JP 2003531208 20031021 JP 2001-578434 20010403 NO 2002004838 20021007 NO 2002-4838 20021007 Α US 2003119842 US 2002-273344 20021018 Α1 20030626 PRIORITY APPLN. INFO.: DE 2000-10019714 A 20000420 WO 2001-EP3772 W 20010403

OTHER SOURCE(S):

MARPAT 135:344484

GΙ

AB Title compds. (ICl-)[II; R1 = CMe3, cyclohexyl, CH2CO2Me, (un)substituted Ph, etc.; R2 = H or alkanoyl; R3 = Me, Ph, 2-furyl, 2-pyridinyl, etc.; R4R5 = (un)substituted CH:CHCH:CH, CH:NCH:CH, N:CHCH:CH, etc.; R8 = (cyclo)alkyl] were prepd. Thus, 2-aminopyridine was cyclocondensed with Me3CNC and PhCHO to give, after N-acylation, II (R1 = CMe3, R2 = H, R3 = Ph, R4R5 = CH:CHCH:CH, R8 = Me). Data for biol. activity of II were given.

# IT 370858-36-9P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses) (prepn. of N-acylimidazopyridineamine chlorides and analogs as  $\mu$ -opiate receptor ligands)

RN 370858-36-9 HCAPLUS

Imidazo[2,1-b]thiazolium, 7-acetyl-5-[(1,1-dimethylethyl)amino]-6-phenyl-,
chloride (9CI) (CA INDEX NAME)

CN

# C1 -

REFERENCE COUNT:

THERE ARE 7 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L8 ANSWER 3 OF 4 HCAPLUS COPYRIGHT 2004 ACS on STN



ACCESSION NUMBER: 2001:283961 HCAPLUS

DOCUMENT NUMBER: 134:295826

TITLE: Preparation of imidazopyridineamines and analogs as

analgesics

INVENTOR(S): Gerlach, Matthias; Maul, Corinna PATENT ASSIGNEE(S): Gruenenthal G.m.b.H., Germany

SOURCE: PCT Int. Appl., 30 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent LANGUAGE: German

FAMILY ACC. NUM. COUNT: 5
PATENT INFORMATION:

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PATENT NO.
                     KIND DATE
                                          APPLICATION NO. DATE
                                           _____
     WO 2001027119
                      A2
                           20010419
                                          WO 2000-EP9098
                                                            20000918
     WO 2001027119
                     A3
                           20011011
         W: AE, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CR, CU,
             CZ, DK, DM, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN,
             IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD,
             MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK,
             SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ,
             BY, KG, KZ, MD, RU, TJ, TM
         RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY,
             DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ,
             CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG
                                         DE 1999-<u>19948434</u> 19991008
     DE 19948434
                      A1
                           20010607
                      Т
                           20030930
                                          PT 2000-969439
     PT 1218378
                                                           20001006
     ZA 2002003579
                      Α
                           20030806
                                          ZA 2002-3579
                                                            20020506
PRIORITY APPLN. INFO.:
                                       DE 1999-19948434 A 19991008
OTHER SOURCE(S):
                        MARPAT 134:295826
GI
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$$\begin{array}{c} Z = Z^{1} \\ R5 \\ R6 \\ NR^{1}R^{2} \\ I \end{array}$$

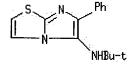
AB Substance libraries comprising, e.g., I [R1 = CMe3, cycloalkyl, (un)substituted Ph, etc.; R2 = H, cycloalkyl, alkanoyl, etc.; R3 = (cyclo)alkyl, (un)substituted (hetero)aryl, etc.; R5,R6 = H, halo, alkyl, alkoxy, etc.; Z = N or CR10; Z1 = N or CR9; R9,R10 = groups cited for R5; Z = N ≠ Z1; Z1 = N ≠ Z] were prepd. Thus, pyridine-2-amine was cyclocondensed with cyclohexanecarboxaldehyde and tert-Bu isocyanide to give I (R1 = CMe3, R2 = R5 = R6 = H, R3 = cyclohexyl, Z = Z1 = CH). Data for biol. activity of I were given.

IT 214531-41-6P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses) (prepn. of imidazopyridineamines and analogs as analgesics)

RN 214531-41-6 HCAPLUS

CN Imidazo[2,1-b]thiazol-5-amine, N-(1,1-dimethylethyl)-6-phenyl- (9CI) (CA INDEX NAME)



L8 ANSWER 4 OF 4 HCAPLUS COPYRIGHT 2004 ACS on STN

Full Citing
Text References
ACCESSION NUMBER:

2001:283960 HCAPLUS

DOCUMENT NUMBER: 134:295829

TITLE:

Preparation of aminoimidazo[2,1-b]thiazoles,

-pyrazoles, and -triazoles as analgesics

INVENTOR(S): Gerlach, Matthias; Maul, Corinna PATENT ASSIGNEE(S): Gruenenthal G.m.b.H., Germany

SOURCE: PCT Int. Appl., 56 pp.

CODEN: PIXXD2

CODEN: PIXXI
OCUMENT TYPE: Patent

DOCUMENT TYPE: LANGUAGE:

German

FAMILY ACC. NUM. COUNT:

PATENT INFORMATION:

| PATENT NO.    |      |                     |      | KI          | DATE | <b>-</b> | APPLICATION NO. DATE |      |   |      |      |            |          |      |      |     |     |
|---------------|------|---------------------|------|-------------|------|----------|----------------------|------|---|------|------|------------|----------|------|------|-----|-----|
| WO 2001027118 |      |                     |      | A2 20010419 |      |          | WO 2000-EP9097       |      |   |      |      |            | 20000918 |      |      |     |     |
| WO            | 2001 | 0271                | 18   | Α           | 3    | 2001     | 0920                 |      |   |      |      |            |          |      |      |     |     |
|               | W:   | ΑE,                 | AL,  | AM,         | ΑT,  | ΑU,      | ΑZ,                  | BA,  | BB,   | BG,  | BR,  | BY,        | CA,      | CH,  | CN,  | CR, | CU, |
|               |      |                     |      |             |      |          |                      |      |   |      |      |            |          | HU,  |      |     |     |
|               |      |                     |      |             |      |          |                      |      |   |      |      |            |          | LU,  |      |     |     |
|               |      |                     |      |             |      |          |                      |      |   |      |      |            |          | SE,  |      |     |     |
|               |      | SL,                 | ТJ,  | TM,         | TR,  | TT,      | TZ,                  | UA,  | UG,   | US,  | UΖ,  | VN,        | ΥU,      | ZA,  | ZW,  | AM, | AZ, |
|               |      | BY,                 | KG,  | ΚZ,         | MD,  | RU,      | ТJ,                  | TM   |   |      |      |            |          |      |      |     | -   |
|               | RW:  | GH,                 | GM,  | ΚE,         | LS,  | MW,      | MZ,                  | SD,  | SL,   | SZ,  | TZ,  | UG,        | ZW,      | ΑT,  | BE,  | CH, | CY, |
|               |      | DE,                 | DK,  | ES,         | FI,  | FR,      | GB,                  | GR,  | ΙE,   | IT,  | LU,  | MC,        | NL,      | PT,  | SE,  | BF, | ВJ, |
|               |      | CF,                 | CG,  | CI,         | CM,  | GΑ,      | GN,                  | GW,  | ML,   | MR,  | NE,  | SN,        | TD,      | TG   |      |     |     |
|               | 1994 |                     |      |             |      |          |                      |      |   |      |      |            |          |      |      |     |     |
|               | 1994 |                     |      |             |      |          |                      |      |   |      |      |            |          |      |      |     |     |
|               |      |                     |      |             |      |          |                      |      | BR 2000-14817 20000918<br>EP 2000-967693 20000918 |      |      |            |          |      |      |     |     |
| EP            |      |                     |      |             |      |          |                      |      |   |      |      |            |          |      |      |     |     |
|               | R:   |                     |      |             |      |          |                      |      |   |      | IT,  | LI,        | LU,      | NL,  | SE,  | MC, | PT, |
|               |      |                     |      |             |      |          | RO,                  |      |   |      |      |            |          |      |      |     |     |
|               | 2003 |                     |      |             |      |          |                      |      |   |      |      |            |          |      |      |     |     |
|               | 2002 |                     |      |             |      |          |                      |      |   |      |      |            |          |      |      |     |     |
|               | 2002 |                     |      |             |      |          |                      |      | <u>U</u>  | S 20 | 02-1 | 1733       | 5        | 2002 | 0408 |     |     |
|               | 6657 |                     |      |             |      |          |                      |      |   |      |      |            |          |      |      |     |     |
|               | 2004 |                     | -    |             | 1    | 2004     | 0205                 |      | U   | S 20 | 03-6 | 33579      | 9        | 2003 | 0805 |     |     |
| ORITY         | APP  | LN.                 | INFO | .:          |      |          |                      |      |   |      |      |            |          | 1999 | +    |     |     |
|               |      |                     |      |             |      |          |                      |      |   |      |      |            |          | 1999 |      |     |     |
|               |      |                     |      |             |      |          |                      |      |   |      |      | ********** |          | 2000 |      |     |     |
|               |      | <i>(</i> ~ <i>)</i> |      |             |      |          |                      |      |   | 002- | 1173 | <u>35</u>  | A3       | 2002 | 0408 |     |     |
| ER SC         | URCE | (S):                |      |             | MAR  | PAT      | 134:2                | 2958 | 29  |      |      |            |          |      |      |     |     |

$$R3$$
 $N$ 
 $N$ 
 $R4$ 
 $R1R2N$ 

I

GΙ

AB Title compds. [I; R1 = CMe3, cyanohexyl, (substituted) Ph, cycloalkyl, etc.; R2 = H, (branched) (substituted) alkylcarbonyl, Ph, naphthyl, pyridyl, thiazolyl, furoyl, etc.; R3 = (branched) alkylcycloalkyl, (substituted) Ph, naphthyl, quinolinyl, anthracenyl, phenanthrenyl, etc.; X = CR5, N, S; Y = N, but when X = S, Y = CR6, N; R4, R5, R6 = H, (branched) alkyl, halo, CF3, cyano, NO2, amino, etc.], were prepd. Using a Zymark robotic synthesis system, 3-amino-1,2,4-triazole and HClO4 in CH2Cl2, furfural in CH2Cl2, and tert-butylisonitrile in CH2Cl2 were added successively to a reactor tube at 15° followed by 11 h stirring at 15° to give tert-butyl-(5-furan-2-yl-imidazo[1,2-b][1,2,4]triazol-6-

```
yl)amine.
                Several I at 10 \muM showed 34-77% \alpha2 adrenoceptor
     affinity.
IT 334771-60-7P
     RL: BAC (Biological activity or effector, except adverse); BSU (Biological
     study, unclassified); SPN (Synthetic preparation); THU (Therapeutic
     use); BIOL (Biological study); PREP (Preparation); USES (Uses)
         (prepn. of aminoimidazothiazoles, -pyrazoles, and -triazoles as
        analgesics)
RN
     334771-60-7 HCAPLUS
CN
     1H-Imidazo[1,2-b][1,2,4]triazol-6-amine, N-(1,1-dimethylethyl)-5-(2-
     furanyl) - (9CI) (CA INDEX NAME)
          NHBu-t
=> d his
     (FILE 'HOME' ENTERED AT 20:57:26 ON 02 MAR 2004)
     FILE 'REGISTRY' ENTERED AT 20:57:31 ON 02 MAR 2004
L1
                STRUCTURE UPLOADED
              0 S L1
L2
L3
              0 S L1 FULL
L4
                STRUCTURE UPLOADED
L_5
              6 S L4
             86 S L4 FULL
L6
     FILE 'HCAPLUS' ENTERED AT 20:59:07 ON 02 MAR 2004
Ь7
             16 S L6
^{P8}
              4 S L6/THU
=> s 16/prep
            16 L6
       3115718 PREP/RL
            13 L6/PREP
                  (L6 (L) PREP/RL)
=> d 19 not 18
L8 IS NOT VALID HERE
For an explanation, enter "HELP DISPLAY".
=> s 19 not 18
L10
             9 L9 NOT L8
=> d l10, ibib abs hitstr, 1-9
L10 ANSWER 1 OF 9 HCAPLUS COPYRIGHT 2004 ACS on STN
            Citing
   Full
ACCESSION NUMBER:
                          2003:363790 HCAPLUS
DOCUMENT NUMBER:
                          139:230677
TITLE:
                         Microwave-assisted multi-component synthesis of fused
                          3-aminoimidazoles
```

Ireland, Sarah M.; Tye, Heather; Whittaker, Mark

Evotec OAI, Abingdon, Oxfordshire, OX14 4SD, UK

AUTHOR (S):

CORPORATE SOURCE:

SOURCE:

Tetrahedron Letters (2003), 44(23), 4369-4371

CODEN: TELEAY; ISSN: 0040-4039

PUBLISHER:

Elsevier Science Ltd.

DOCUMENT TYPE:

Journal

LANGUAGE:

English

OTHER SOURCE(S):

CASREACT 139:230677

A variety of fused 3-aminoimidazoles have been synthesized by a microwave assisted Ugi three-component coupling (3cc) reaction catalyzed by scandium triflate in methanol as solvent. Yields of 33-93% have been achieved after just 10 min of microwave irradn. using a simple one-stage procedure. The methodol. described is suitable for the rapid and efficient synthesis of a range of fused heterocycles of pharmacol. interest.

IT 593270-92-9P

RL: SPN (Synthetic preparation); PREP (Preparation)

(synthesis of fused 3-aminoimidazoles via microwave assisted Ugi three-component coupling as the key step)

593270-92-9 HCAPLUS RN

Imidazo[2,1-b]thiazol-5-amine, 6-(2-naphthalenyl)-N-(phenylmethyl)- (9CI) CN (CA INDEX NAME)

- CH 2-- Ph

REFERENCE COUNT:

THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

ANSWER 2 OF 9 HCAPLUS COPYRIGHT 2004 ACS on STN

Full Text References

ACCESSION NUMBER:

2003:90593 HCAPLUS

DOCUMENT NUMBER:

138:401653

TITLE:

Fused heterocycles: Synthesis of some new

imidazothiazoles

AUTHOR (S):

Cesur, Nesrin; Cesur, Zafer; Guner, Handan;

Kasimogullari, B. Ozden

CORPORATE SOURCE:

Department of Pharmaceutical Chemistry, Faculty of

Pharmacy, University of Istanbul, Instanbul, 34452,

Turk.

SOURCE:

Heterocyclic Communications (2002), 8(5), 433-438

II.

CODEN: HCOMEX; ISSN: 0793-0283

PUBLISHER: DOCUMENT TYPE: Freund Publishing House Ltd.

Journal

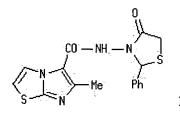
LANGUAGE:

English

OTHER SOURCE(S):

CASREACT 138:401653

GI



AB Reaction of aldehyde-hydrazones or semicarbazones bearing an imidazo[2,1-b][1,3]thiazole ring system with mercaptoalkanoic acids were investigated and found to give thiazolidine and thiazine derivs., e.g. I and II. Antimycobacterial activities of compds. thus obtained were evaluated against Mycobacterium tuberculosis H37Rv using rifampine as std. (no data).

### IT 531501-57-2P 531501-58-3P 531501-59-4P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP

(Preparation); RACT (Reactant or reagent)

(synthesis of some new imidazothiazoles via aldehyde hydrazones or semicarbazones)

RN 531501-57-2 HCAPLUS

CN Carbamic acid, (6-methylimidazo[2,1-b]thiazol-5-yl)-, ethyl ester (9CI) (CA INDEX NAME)

RN 531501-58-3 HCAPLUS

CN Hydrazinecarboxamide, N-(6-methylimidazo[2,1-b]thiazol-5-yl)- (9CI) (CA INDEX NAME)

RN 531501-59-4 HCAPLUS

CN Hydrazinecarboxamide, N-(6-methylimidazo[2,1-b]thiazol-5-yl)-2-(phenylmethylene)- (9CI) (CA INDEX NAME)

# IT 531501-60-7P 531501-73-2P 531501-74-3P

RL: SPN (Synthetic preparation); PREP (Preparation)

(synthesis of some new imidazothiazoles via aldehyde hydrazones or semicarbazones)

RN 531501-60-7 HCAPLUS

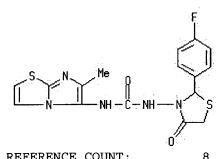
CN Urea, N-(6-methylimidazo[2,1-b]thiazol-5-yl)-N'-(4-oxo-2-phenyl-3-thiazolidinyl)- (9CI) (CA INDEX NAME)

RN 531501-73-2 HCAPLUS

CN Hydrazinecarboxamide, 2-[(4-fluorophenyl)methylene]-N-(6-methylimidazo[2,1-b]thiazol-5-yl)- (9CI) (CA INDEX NAME)

531501-74-3 HCAPLUS RN

CN Urea, N-[2-(4-fluorophenyl)-4-oxo-3-thiazolidinyl]-N'-(6-methylimidazo[2,1b]thiazol-5-yl)- (9CI) (CA INDEX NAME)



REFERENCE COUNT:

THERE ARE 8 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

ANSWER 3 OF 9 HCAPLUS COPYRIGHT 2004 ACS on STN

References

2000:211394 HCAPLUS ACCESSION NUMBER:

DOCUMENT NUMBER: 132:334420

TITLE:

Synthesis of new functionalized imidazo[2,1b]thiazoles and thiazolo[3,2-a]pyrimidines

Peterlin-Masic, Lucija; Malesic, Mateja; Breznik, AUTHOR (S):

Matej; Krbavcic, Ales

CORPORATE SOURCE: Faculty of Pharmacy, University of Ljubljana,

Ljubljana, 1000, Slovenia

SOURCE: Journal of Heterocyclic Chemistry (2000), 37(1),

CODEN: JHTCAD; ISSN: 0022-152X

PUBLISHER: HeteroCorporation

DOCUMENT TYPE: Journal LANGUAGE: English

5-0xo-5H-[1,3]thiazolo[3,2-a]pyrimidine-6-carboxylic acid and 6-methylimidazo[2,1-b]thiazole-5-carboxylic acid were reacted with amines via reaction with oxalyl chloride and use of N,N-dimethylformamide as a catalyst to give primary and secondary amide derivs. N,N'-disubstituted ureas and perhydroimidazo[1,5-c]thiazole derivs. of imidazo[2,1-b]thiazole were also prepd. By NMR anal. of one of the compds. prepd., existence of two stereoisomers resulting from both optical and conformational isomerism was obsd.

IT 267897-75-6P 267897-76-7P

RL: SPN (Synthetic preparation); PREP (Preparation)

(prepn. of imidazo[2,1-b]thiazoles and thiazolo[3,2-a]pyrimidines)

267897-75-6 HCAPLUS RN

Glycine, N-[[(6-methylimidazo[2,1-b]thiazol-5-yl)amino]carbonyl]-, ethyl ester (9CI) (CA INDEX NAME)

CN L-Alanine, N-[[(6-methylimidazo[2,1-b]thiazol-5-yl)amino]carbonyl]-, methyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

REFERENCE COUNT:

THERE ARE 21 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

Marrow

L10 ANSWER 4 OF 9 HCAPLUS COPYRIGHT 2004 ACS on STN

21

Full Citing Text References

ACCESSION NUMBER:

1998:624858 HCAPLUS

DOCUMENT NUMBER:

129:302566

TITLE:

A new heterocyclic multicomponent reaction for the combinatorial synthesis of fused 3-aminoimidazoles

Bienayme, Hugues; Bouzid, Kamel

CORPORATE SOURCE:

Rhone-Poulenc Technologies, St-Fons, F-69192, Fr.

SOURCE:

AUTHOR(S):

Angewandte Chemie, International Edition (1998),

37(16), 2234-2237

CODEN: ACIEF5; ISSN: 1433-7851

PUBLISHER:

Wiley-VCH Verlag GmbH

DOCUMENT TYPE:

Journal

LANGUAGE:

English

OTHER SOURCE(S):

CASREACT 129:302566

GI

N N

INCM- 7

AB Reaction of heteroarom. amidines, aldehydes, and isonitriles in the presence of a catalytic amt. of protic acids gave fused 3-aminoimidazoles. E.g., HClO4-catalyzed reaction of 2-aminopyrimidine, PhCHO, and Me3CNC gave 82% imidazopyrimidine I.

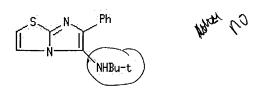
IT 214531-41-6P 214531-42-7P 214531-43-8P

214531-45-0P 214531-46-1P

RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of fused aminoimidazoles by multicomponent reaction of aminoamidines, aldehydes, and isonitriles)

RN 214531-41-6 HCAPLUS

CN Imidazo[2,1-b]thiazol-5-amine, N-(1,1-dimethylethyl)-6-phenyl- (9CI) (CA INDEX NAME)



RN 214531-42-7 HCAPLUS

CN Imidazo[2,1-b]thiazole-3-acetic acid, 5-[(1,1-dimethylethyl)amino]-6-phenyl-, ethyl ester (9CI) (CA INDEX NAME)

t-Bunh CH 2-C-OEt

RN 214531-43-8 HCAPLUS

CN Imidazo[2,1-b]-1,3,4-thiadiazol-5-amine, N-(1,1-dimethylethyl)-6-phenyl-(9CI) (CA INDEX NAME)

NHBu-t

RN 214531-45-0 HCAPLUS

CN TH-Imidazo[1,2-b][1,2,4]triazol-6-amine, N-(1,1-dimethylethyl)-5-phenyl-(9CI) (CA INDEX NAME)

NHBu-t

RN 214531-46-1 HCAPLUS

CN 5H-Imidazo[1,2-b]pyrazole-7-carboxylic acid, 3-[(1,1-dimethylethyl)amino]-2-phenyl-, ethyl ester (9CI) (CA INDEX NAME)

Ph NHBu-t

REFERENCE COUNT:

32 THERE ARE 32 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L10 ANSWER 5 OF 9 HCAPLUS COPYRIGHT 2004 ACS on STN

Full Citing
Text References

ACCESSION NUMBER: 1997:169046 HCAPLUS

DOCUMENT NUMBER: 126:238333

TITLE: Transformations of methyl L-(-)-Thiazolidine-4-

carboxylate, 2-amino-2-thiazoline and 2-aminothiazole

into thiazoloazines and azolothiazoles

AUTHOR(S): Malesic, Mateja; Krbavcic, Ales; Stanovnik, Branko

CORPORATE SOURCE: Faculty of Pharmacy, University of Ljubljana,

Lujbljana, 1000, Slovenia

SOURCE: Journal of Heterocyclic Chemistry (1997), 34(1), 49-55

CODEN: JHTCAD; ISSN: 0022-152X

PUBLISHER: HeteroCorporation

DOCUMENT TYPE: Journal

PD400.114

3/2/04

LANGUAGE:

English

In the search for potential immunomodulators Me L-(-)-thiazolidine-4-AB carboxylate (I), 2-amino-2-thiazoline (II), and 2-aminothiazole (III) were transformed into derivs. of various bicyclic systems. Thus, from I, derivs. of perhydrothiazolo[3,4-a]pyrazine, perhydrothiazolo[4,3c] [1,4] oxazine, and perhydroimidazo[1,5-c] thiazole were prepd. From II, derivs. of 2,3-dihydrothiazolo[2,3-b]pyrimidine were prepd. From III, derivs. of imidazo[2,1-b]thiazoline were prepd. 6-(P-Sulfamoylphenyl)-7oxoperhydroimidazo[1,5-c]thiazole-5-thione was found to exhibit immunorestoration activity.

IT 188561-50-4P 188561-52-6P 188561-59-3P

RL: SPN (Synthetic preparation); PREP (Preparation)

(transformations of Me thiazolidinecarboxylate, aminothiazoline, and aminothiazole into thiazoloazines and azolothiazoles)

188561-50-4 HCAPLUS RN

Urea, (6-methylimidazo[2,1-b]thiazol-5-yl)- (9CI) (CA INDEX NAME) CN

188561-52-6 HCAPLUS RN

Urea, N,N'-bis(6-methylimidazo[2,1-b]thiazol-5-yl)- (9CI) (CA INDEX NAME) CN

RN 188561-59-3 HCAPLUS

Urea, N-(4,5-dimethyl-2-oxazolyl)-N'-(6-methylimidazo[2,1-b]thiazol-5-yl)-CN(9CI) (CA INDEX NAME)

REFERENCE COUNT:

THERE ARE 17 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

ANSWER 6 OF 9 HCAPLUS COPYRIGHT 2004 ACS on STN L10

17

Full Liting <u>References</u> Text

ACCESSION NUMBER:

TITLE:

1987:102158 HCAPLUS

DOCUMENT NUMBER:

106:102158

Novel syntheses of fused imidazoles. III. Simplified construction of the imidazo[2,1-b]thiazoline system

Lantos, Ivan; McGuire, Michael AUTHOR(S):

Chem. Res. Dev., Smith Kline and French Lab., CORPORATE SOURCE:

Philadelphia, PA, 19101, USA

Heterocycles (1986), 24(4), 991-6 SOURCE:

CODEN: HTCYAM; ISSN: 0385-5414

DOCUMENT TYPE:

Journal

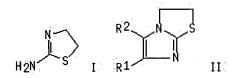
LANGUAGE:

English

OTHER SOURCE(S):

CASREACT 106:102158

G3



AB Aminothiazoline I reacted with 4-RC6H4CHO (R = OMe, F, H, Me) in the presence of NaCN at room temp. to give imidazothiazolines II (R1 = 4-RC6H4; R2 = R1CH:N) in 20-80% yields. Acid hydrolysis of the latter gave II (R2 = NH2).

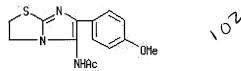
IT 106726-46-9P 106745-03-3P

RL: SPN (Synthetic preparation); PREP (Preparation)

(prepn. of)

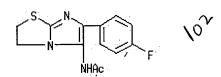
RN 106726-46-9 HCAPLUS

CN Acetamide, N-[2,3-dihydro-6-(4-methoxyphenyl)imidazo[2,1-b]thiazol-5-yl](9CI) (CA INDEX NAME)



RN 106745-03-3 HCAPLUS

CN Acetamide, N-[6-(4-fluorophenyl)-2,3-dihydroimidazo[2,1-b]thiazol-5-yl](9CI) (CA INDEX NAME)



L10 ANSWER 7 OF 9 HCAPLUS COPYRIGHT 2004 ACS on STN

Full Citing Text References

ACCESSION NUMBER: 1974:505382 HCAPLUS

DOCUMENT NUMBER: 81:105382

TITLE: Cyclization of ω-chloro-ω-acylamido

acetophenones

AUTHOR(S): Drach, B. S.; Dolgushina, I. Yu.; Sinitsa, A. D.

CORPORATE SOURCE: Inst. Org. Khim., Kiev, USSR

SOURCE: Khimiya Geterotsiklicheskikh Soedinenii (1974), (7),

928-31

CODEN: KGSSAQ; ISSN: 0132-6244

DOCUMENT TYPE:

Journal

LANGUAGE: Russian

GI For diagram(s), see printed CA Issue.

AB Acylamidothiazoles (I; R = Me, MeO, Ph, PhCH2O; R1 = H, Ph, MeS, NH2, Me) were obtained in 60-94% yields by cyclization of RCONHCHClCOPh (II) with R1CSNH2 1 hr in boiling THF. Analogously obtained were 60-86% benzothiazines (III; R = Me, Ph, MeO) from o-aminobenzenethiol, 55-62%

imidazothiazoles (IV; R = Me, MeO) from 2-aminothiazole, and 60-8%

imidazopyridines (V; R = Me, MeO) from 2-aminopyridine.

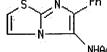
IT 54167-97-4P 54167-98-5P

RL: SPN (Synthetic preparation); PREP (Preparation)

(prepn. of)

RN 54167-97-4 HCAPLUS

CN Acetamide, N-(6-phenylimidazo[2,1-b]thiazol-5-yl)- (9CI) (CA INDEX NAME)



102

RN 54167-98-5 HCAPLUS

CN Carbamic acid, (6-phenylimidazo[2,1-b]thiazol-5-yl)-, methyl ester (9CI) (CA INDEX NAME)

L10 ANSWER 8 OF 9 HCAPLUS COPYRIGHT 2004 ACS on STN

Full Citing Text References

ACCESSION NUMBER: 1973:159516 HCAPLUS

DOCUMENT NUMBER: 78:159516

TITLE: 1H-Imidazo[1,2-a]imidazoles. II. Chemistry of

1,6-dimethyl-1H-imidazo[1,2-a]imidazole

AUTHOR(S): Miller, Laird F.; Bambury, Ronald E.

CORPORATE SOURCE: Merrell-Natl. Lab. Div., Richardson-Merrell, Inc.,

Cincinnati, OH, USA

SOURCE: Journal of Organic Chemistry (1973), 38(10), 1955-7

CODEN: JOCEAH; ISSN: 0022-3263

DOCUMENT TYPE: Journal LANGUAGE: English

OTHER SOURCE(S): CASREACT 78:159516
GI For diagram(s), see printed CA Issue.

AB Electrophilic substitutions of 1,6-dimethyl-1H-imidazo [1,2-a]imidazole (I) occurred initially at the 5-position. Nitration of I also gave a dinitrated product whose structure was not conclusively established. A series of Hueckel MO calcns. were made in order to det. the site of substitution.

IT 38739-98-9P 38739-99-0P

RL: SPN (Synthetic preparation); PREP (Preparation) (prepn. of)

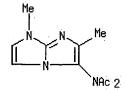
RN 38739-98-9 HCAPLUS

CN Acetamide, N-(1,6-dimethyl-1H-imidazo[1,2-a]imidazol-5-yl)- (9CI) (CA INDEX NAME)

RN 38739-99-0 HCAPLUS

CN Acetamide, N-acetyl-N-(1,6-dimethyl-1H-imidazo[1,2-a]imidazol-5-yl)- (9CI)

#### (CA INDEX NAME)



ANSWER 9 OF 9 HCAPLUS COPYRIGHT 2004 ACS on STN

Citing References

ACCESSION NUMBER: 1968:95754 HCAPLUS

DOCUMENT NUMBER: 68:95754

TITLE: Substitution and addition reactions of

2-phenylimidazo[2,1-b]benzothiazole

Pentimalli, Luciano; Guerra, Anna Marià AUTHOR (S):

Univ. Bologna, Bologna, Italy CORPORATE SOURCE:

Gazzetta Chimica Italiana (1967), 97(8), 1286-93 SOURCE:

CODEN: GCITA9; ISSN: 0016-5603

DOCUMENT TYPE: Journal LANGUAGE: Italian

GI For diagram(s), see printed CA Issue.

AΒ Compds. of the general formulas I and II are prepd. A mixt. of 3.3 q. 2-amino-4-methylthiazole, 6 g. BrCH2COPh, and 30 ml. EtOH is refluxed 3 hrs. to give 68% 3-methyl-6-phenylimidazo[2,1-b]thiazole (III), m. 113° (ligroine). Similarly prepd. are (m.p. given): 2-phenylimidazo[2,1-b]-benzothiazole (IV), 97-9° (HCl salt m.  $224-6^{\circ}$ ); I (Y = H, X = NO2),  $257-8^{\circ}$  (pyridine); II (Y = H, X = NO2), 284-6°. A mixt. of 1 g. IV, 0.8 g. EtO2CN:NCO2Et, and 15 ml. C6H6 is refluxed 3 hrs. to give 90% II [X = H, Y = N(CO2Et)NHCO2Et], m. 172-3° (C6H6-ligroine). Similarly prepd. is I [X = H, Y = N(CO2Et)NHCO2Et], m. 143° (C6H6-ligroine). A mixt. of 1 g. III, 0.45 g. maleic anhydride, and 45 ml. C6H6 is refluxed to give 91% I [X =H, Y = CH(CO2H)CH2CO2H, m. 179-80° (EtOH). Similarly prepd. is II [X = H, Y = CH(CO2H)CH2CO2H], m. 173-4° (xylene). A mixt. of 1 q. IV, diazonium salt (prepd. from 0.6 g. p-O2NC6H4NH2), and 20 ml. pyridine is kept overnight to give II (X = H, Y = p-O2NC6H4N:N), m. 240-1° (HOAc). Similarly prepd. is I (X = H, Y = p-02NC6H4N:N), m. 171-2° (ligroine). A soln. of 1 g. IV in 10 ml. HOAc is treated with an aq. soln. of 0.5 g. NaNO2, the mixt. agitated 30 min., and neutralized with 10% NaOH to give 52% II (X = H, Y = NO), m. 179-80° (ligroin). A soln. of 2 g. IV in 20 ml. concd. H2SO4 is cooled, treated with 0.8 ml. HNO3 (d. 1.40), and agitated 90 min. to give II (X = Y = NO2), m.  $327-9^{\circ}$ , and II (X = NO2, Y = H), m.  $282-5^{\circ}$  (pyridine).

Similarly prepd. is I (X = Y = NO2), m. 289-90° (pyridine).

IT 17833-09-9P

RL: SPN (Synthetic preparation); PREP (Preparation) (prepn. of)

17833-09-9 HCAPLUS RN

CN Bicarbamic acid, (3-methyl-6-phenylimidazo[2,1-b]thiazol-5-yl)-, diethyl ester (8CI) (CA INDEX NAME)

=> d his

(FILE 'HOME' ENTERED AT 20:57:26 ON 02 MAR 2004)

FILE 'REGISTRY' ENTERED AT 20:57:31 ON 02 MAR 2004

L1 STRUCTURE UPLOADED

L2 0 S L1

L3 0 S L1 FULL

L4 STRUCTURE UPLOADED

L5 6 S L4

L6 86 S L4 FULL

FILE 'HCAPLUS' ENTERED AT 20:59:07 ON 02 MAR 2004

L7 16 S L6

L8 4 S L6/THU

L9 13 S L6/PREP

L10 9 S L9 NOT L8

=> s 17 not 19

L11 3 L7 NOT L9

=> d 111, ibib abs fhitstr, 1-3

L11 ANSWER 1 OF 3 HCAPLUS COPYRIGHT 2004 ACS on STN

Full Citing Text References

ACCESSION NUMBER: 1995:350430 HCAPLUS

DOCUMENT NUMBER: 122:147044

TITLE: A silver halide color photographic material.

INVENTOR(S): Ikesu, Satoru; Kaneko, Yutaka PATENT ASSIGNEE(S): Konica Corporation, Japan SOURCE: Eur. Pat. Appl., 37 pp.

CODEN: EPXXDW

DOCUMENT TYPE:

Patent

LANGUAGE:

English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

| PATENT NO.           | KIND      | DATE         |     | APPLICATION NO. | DATE     |
|----------------------|-----------|--------------|-----|-----------------|----------|
|                      |           | ~            |     |                 |          |
| EP 608133            | <b>A1</b> | 19940727     |     | EP 1994-300429  | 19940120 |
| EP 608133            | В1        | 19990707     |     |                 |          |
| R: DE, FR,           | GB, NL    |              |     |                 |          |
| JP 06222526          | A2        | 19940812     |     | JP 1993-8572    | 19930121 |
| JP 06242569          | A2        | 19940902     |     | JP 1993-25720   | 19930215 |
| JP 06242570          | A2        | 19940902     |     | JP 1993-25721   | 19930215 |
| PRIORITY APPLN. INFO | . :       |              | JΡ  | 1993-8572       | 19930121 |
|                      |           |              | JP  | 1993-25720      | 19930215 |
|                      |           |              | JP  | 1993-25721      | 19930215 |
| OTHER SOURCE(S):     | MA        | RPAT 122:147 | 044 |                 |          |

AΒ A Ag halide color photog. material comprises ≥1 of the hydrophilic colloid layers contg. a cyan dye-forming coupler represented by I, II, or III [R1-R3, Y = H, substituent; EWG = electron withdrawing group having Hammet's substituent const. ≥0.3; X = H, group capable of splitting off upon reaction with an oxidized product of a color developing agent]. The formed dye images have improved hue stability against heat, moisture and light.

#### IT 160877-96-3

RL: DEV (Device component use); TEM (Technical or engineered material use); USES (Uses)

(photog. cyan coupler for improved hue stability)

RN 160877-96-3 HCAPLUS

CN Heneicosanoic acid, 3-[[[6-[(butylamino)sulfonyl]-2-methyl-1H-imidazo[1,2a]imidazol-3-yl]amino]carbonyl]- (9CI) (CA INDEX NAME)

ANSWER 2 OF 3 HCAPLUS COPYRIGHT 2004 ACS on STN

References Text ACCESSION NUMBER:

1993:222791 HCAPLUS

DOCUMENT NUMBER: 118:222791

TITLE: Photographic cyan coupler with heat and moisture

resistance

INVENTOR(S): Kita, Hiroshi; Kaneko, Yutaka; Ikesu, Satoru

PATENT ASSIGNEE(S): Konica Co., Japan

SOURCE: Jpn. Kokai Tokkyo Koho, 14 pp.

CODEN: JKXXAF DOCUMENT TYPE: Patent

LANGUAGE:

Japanese

FAMILY ACC. NUM. COUNT:

PATENT INFORMATION:

| PATENT NO.            | KIND | DATE          | APPLICATION NO. | DATE     |
|-----------------------|------|---------------|-----------------|----------|
|                       |      |               |                 |          |
| JP 04260035           | A2   | 19920916      | JP 1991-42345   | 19910215 |
| JP 2849954            | B2   | 19990127      |                 |          |
| PRIORITY APPLN. INFO. | :    |               | JP 1991-42345   | 19910215 |
| OTHER SOURCE(S):      | MA   | RPAT 118:2227 | 91              |          |

GI

$$R^1$$
 $R^2$ 
 $R^3$ 
 $R^3$ 

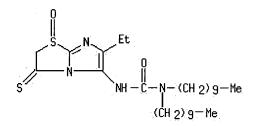
AB Photog. coupler I (R1-2 = H, substituent, R1 and R2 may form a ring; R3 = H, releasing group by the reaction with the oxidized color developing agent; Z = 0, S; n = 1-2). The coupler gives cyan images with heat-, light-, and moisture-resistance.

IT 147034-73-9

RL: TEM (Technical or engineered material use); USES (Uses) (photog. cyan coupler)

RN 147034-73-9 HCAPLUS

CN Urea, N,N-didecyl-N'-(6-ethyl-2,3-dihydro-1-oxido-3-thioxoimidazo[2,1-b]thiazol-5-yl)- (9CI) (CA INDEX NAME)



L11 ANSWER 3 OF 3 HCAPLUS COPYRIGHT 2004 ACS on STN

Full Citing
Text References

ACCESSION NUMBER: 1963:14863 HCAPLUS

DOCUMENT NUMBER: 58:14863

ORIGINAL REFERENCE NO.: 58:2443e-h,2444a-e

TITLE: Bicyclic heterocyclic compounds with a common nitrogen

atom. IV. Aminoimidazo[2,1-b]thiazoles

AUTHOR(S): Pyl, Theodor; Wuensch, Karl Heinz; Buelling, Lothar;

Beyer, Hans

CORPORATE SOURCE: Univ. Greifswald, Germany SOURCE: Ann. (1962), 657, 113-20

DOCUMENT TYPE: Journal LANGUAGE: Unavailable

5-Nitro- (I) and 5-nitrosoimidazo[2,1-b]thiazoles (II) were reduced with In in AcOH to give the corresponding 5-NH2 derivs. (III), which were relatively stable and behaved chem. as aromatic amines. I were dissolved or suspended in AcOH, treated portionwise with Zn dust with gentle heating, filtered, and the filtrate treated with Et20-HCl or a few drops concd. H2SO4 [in the latter case the initially formed ppt. (ZnSO4) was discarded; the product crystd. on standing] gave III HCl or H2SO4 salts. Treatment of III salts in H2O with satd. aq. NaOAc or aq. picric acid (IV) gave free III and III picrates, resp. The following III were prepd. in this manner [R, R', R''', m.p. (decompn.), recrystn. solvent, % yield given] (R'' = H in all cases): H, H, Br (V), 183° dil. EtOH, 50; Me, H, Br (VI), 217°, MeOH, 20; H, Me, Br (VII), 200°, MeOH, 50; Me, Me, Br (VIII), 220° MeOH, 20; H, H, Cl (IX), 206°, dil. EtOH, 50; H, H, Me (as picrate), 250° (unsharp), aq. IV, 30; H, H, NH2 (as tri-HCl salt), above 300°, dil. HCl, 70; Me, H, NH2 (as dipicrate), 223°, --, 75; H, Me, NH2 (as dipicrate),

196°, alc.-IV, 65. II dissolved or suspended in AcOH cooled until the greater part of the AcOH solidified, treated portionwise with Zn dust with stirring, when decolorized the soln. filtered, the filtrate treated with a few drops concd. H2SO4 [the initial ppt. (ZnSO4) was discarded], and kept several hrs. gave III sulfate, converted to the free base or picrate as above. Thus were prepd. the following III (same data as above given) (R'' = H in all cases): H, H, Br, 183°, --, --; H, H, H (as picrate), 234°, aq. IV, 40; H, Me, H (as picrate), 213°, --, 33. The bases V-IX were stable; the other bases were unstable and were isolated only as picrates. 5-Nitro-6-(p-bromophenyl)imidazo[2,1b]thiazole (1.6 g.) in 10 cc. AcOH and 5 cc. Ac2O treated with Zn dust and dild. with H2O gave 1.3 g. III (R'' = Ac, R = R' = H, R''' = Br), m. 211° (decompn.) (dil. EtOH). V (1 g.), 0.9 g. 4-EtO2CNHC6H4SO2Cl, and 0.3 g. pyridine in 100 cc. MeOH heated 2 hrs. and cooled gave 1.1 q. III (R = R' = H, R'' = 4-EtO2CNHC6H4SO2, RH''' = Br) (X) hydrate, m. 195° (H2O); X.HO2 dried in vacuo at 110° gave anhyd. X, m. 214-15°. X (1 g.) and 2 cc. 2N EtOH-NaOH in 50 cc. EtOH heated 6 hrs. at 60°, concd., poured into 1 l. H2O, and kept several hrs. gave 0.6 g. III (R = R' = H, R'' = 4-H2NC6H4SO2, R''' = Br), m. 210-11°. V (1.5 g.) in 75 cc. Me2CO treated with 2 g. PhNCO, kept 1 hr., and concd. gave 1.7 g. III (R = R' = H, R'' = PhNHCO, R''' = Br), m. 238° (decompn.) (EtOH). V (1.5 q.) and 0.7 q. PhNCS treated with 1 drop pyridine, heated (exothermic reaction), the melt taken up in EtOH, and the soln. treated with H2O gave 1.3 g. III (R = R' = H, R'' = PhNHCS, R''' = Br), m. 202° (decompn.) (dil. EtOH). V (1.5 g.) and 5 cc. BzH heated 5 min., the product dissolved in EtOH, and the soln. treated with H2O gave 1.2 g. benzylidene deriv. of V, m. 195° (decompn.) (EtOH). V (1.5 g.) and 3 cc. 2-HOC6H4CHO treated similarly gave 1.1 q. salicylidene deriv. of V, m. 215° (decompn.) (EtOH with C). V (2.9 g.) in 10 cc. concd. HCl and 100 cc. H2O treated with 0.8 g. NaNO2 at 0-5° and the ppt. filtered off rapidly gave moist III (R = R' = R'' = ON, R''' = Br) (XI). Freshly prepd. moist XI suspended in 20 cc. AcOH treated with Zn dust, the resulting light yellow soln. heated 5 min. with 1 cc. BzH, dild. with EtOH, treated with H2O, and kept overnight gave 0.1 g. III (R = R' = R'' = PhCH:N, R''' = Br), m. 210-11° (decompn.)(dil. EtOH). V (1.5 g.) in 15 cc. 50% HBr treated with 0.4 g. NaNO2 at 0-5° and the resulting diazonium soln. coupled with 2-naphthol gave XII. 2,4-Diaminothiazole and 4 g. BzCH2Br (XIII) in 250 cc. EtOH kept 1 hr. deposited 2.5 g. XIV (R = NH2), m. 244° (decompn.) (H2O with C). XIV (R = NH2) (1.5 g.) heated 2 hrs. with concd. HBr and cooled deposited 0.7 g. XIV (R = OH), m. 212° (decompn.) (EtOH). XIV (R = OH) NH2) (3.1 g.) dissolved in 200 cc. boiling H2O, the soln. treated with satd. aq. NaOAc, the resinous product dissolved in EtOH, and the soln. treated with 1 cc. concd. HNO3 gave 2.5 g. 3-hydroxy-6-phenylimidazo [2,1-b]thiazole, m. 183° (decompn.). 2-Amino-4-methyl-5carbethoxythiazole (3.7 g.) and 4 g. XIII in 50 cc. EtOH heated 30 hrs., cooled, the ppt. filtered off, suspended in H2O, and the suspension heated with NaOAc and cooled gave 4.7 g. XV (R = OEt), m.  $144-5^{\circ}$  (EtOH). XV (R = OEt) (1.4 g.) and 1 cc. 100% N2H4.H2O in 10 cc. EtOH heated 10 hrs. at  $70^{\circ}$  and cooled gave 0.9 g. XV (R = NHNH2) (XVI), m.235° (EtOH). XVI (1.4 g.) in 8 cc. AcOH treated with 0.4 g. NaNO2 and dild. with 100 cc. H20 gave 1 g. XV (R = N3), decompd. when heated. XV (R = N3) (1.4 g.) in 15 cc. AcOH and 15 cc. Ac2O heated until N evolution ceased, poured into 400 cc. H2O, and treated dropwise with 2N NaOH until a flocculent ppt. sepd. gave 0.7 g. 2-acetamido-3-methyl-6phenylimidazo [2, 1-b] thiazole, m. 225° (decompn.) (EtOH with C). IT 92905-61-8, Imidazo[2,1-b]thiazole, 5-acetamido-6-(p-bromophenyl)-(prepn. of) 92905-61-8 HCAPLUS Imidazo[2,1-b]thiazole, 5-acetamido-6-(p-bromophenyl)- (7CI) (CA INDEX

RN

CN

NAME)

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### => d his

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FILE 'REGISTRY' ENTERED AT 20:57:31 ON 02 MAR 2004
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L3 0 S L1 FULL
L4 STRUCTURE UPLOADED

L5 6 S L4 L6 86 S L4 FULL

FILE 'HCAPLUS' ENTERED AT 20:59:07 ON 02 MAR 2004

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L8 4 S L6/THU
L9 13 S L6/PREP
L10 9 S L9 NOT L8
L11 3 S L7 NOT L9

FILE 'CAOLD' ENTERED AT 21:04:05 ON 02 MAR 2004

=> s 16

L12

2 L6

=> d 112, all, 1-2

L12 ANSWER 1 OF 2 CAOLD COPYRIGHT 2004 ACS on STN

AN / CA58:2443e CAOLD

FI bicyclic heterocyclic compds with a common N atom - (IV) aminoimidazo[2,1-b]thiazoles

AU Pyl, Theodor; Wuensch, K. H.; Buelling, L.; Beyer, H.

 IT
 74416-91-4
 88855-97-4
 88855-99-6
 91183-08-3
 91394-83-1
 91394-84-2

 91635-13-1
 92286-32-3
 92545-85-2
 93327-30-1
 93819-53-5
 93869-37-5

 94463-22-6
 94574-43-3
 94622-88-5
 94802-80-9
 94802-82-1
 94994-64-6

 95315-23-4
 95315-26-7
 96984-80-4
 96986-17-3
 97026-49-8
 111164-78-4

L12 ANSWER 2 OF 2 CAOLD COPYRIGHT 2004 ACS on STN

AN CA56:2442g CAOLD

TI phenoxazines - (V) syntheses of 7-amino-2-phenoxazones

AU Musso, Hans; Wager, P.

IT 493-42-5 1916-58-1 2835-97-4 3950-31-0 26103-30-0 26103-31-1 53669-94-6 53669-95-7 53669-97-9 67862-51-5 92060-74-7 92102-80-2 92149-10-5 92149-30-9 92149-31-0 92437-82-6 92873-56-8 92905-61-8 93014-15-4 93431-78-8 93986-16-4 94538-61-1 94709-90-7 94906-40-8 95019-65-1 98016-21-8 98396-82-8

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ANSWER 1 REGISTRY COPYRIGHT 2004 ACS on STN

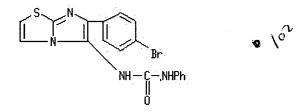
RN 95315-23-4 REGISTRY

CN Urea, 1-[6-(p-bromophenyl)imidazo[2,1-b]thiazol-5-yl]-3-phenyl- (7CI) (CA INDEX NAME)

FS 3D CONCORD

MF C18 H13 Br N4 O S

LC STN Files: BEILSTEIN\*, CA, CAOLD, CAPLUS
(\*File contains numerically searchable property data)



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

- 1 REFERENCES IN FILE CA (1907 TO DATE)
- 1 REFERENCES IN FILE CAPLUS (1907 TO DATE)
- 1 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

FILE 'CAOLD' ENTERED AT 21:04:21 ON 02 MAR 2004

=> fil reg; d acc 95315-26-7; fil CAOLD

FILE 'REGISTRY' ENTERED AT 21:04:23 ON 02 MAR 2004

ANSWER 1 REGISTRY COPYRIGHT 2004 ACS on STN

RN 95315-26-7 REGISTRY

CN Urea, 1-[6-(p-bromophenyl)imidazo[2,1-b]thiazol-5-yl]-3-phenyl-2-thio-(7CI) (CA INDEX NAME)

FS 3D CONCORD

MF C18 H13 Br N4 S2

LC STN Files: BEILSTEIN\*, CA, CAOLD, CAPLUS

(\*File contains numerically searchable property data)

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- 1 REFERENCES IN FILE CAPLUS (1907 TO DATE)
- 1 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

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=> fil reg; d acc 92905-61-8; fil CAOLD

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ANSWER 1 REGISTRY COPYRIGHT 2004 ACS on STN

RN 92905-61-8 REGISTRY

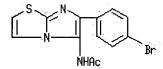
CN Imidazo[2,1-b]thiazole, 5-acetamido-6-(p-bromophenyl)- (7CI) (CA INDEX NAME)

FS 3D CONCORD

MF C13 H10 Br N3 O S

LC STN Files: BEILSTEIN\*, CA, CAOLD, CAPLUS

(\*File contains numerically searchable property data)



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)
1 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

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|  | ENTRY      | SESSION |
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